Investigation of the Microstructure of Micelles Formed by Hard-Sphere Chains Interacting via Size Nonadditivity by Discontinuous Molecular Dynamics Simulation.

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Abstract

Micelle formation by short nonadditive hard surfactant chains was investigated at different size ratios, reduced densities, and nonadditivity parameters using mol. dynamics simulation. It was found that spherical, cylindrical, lamellar, and reverse micelles can form in systems with different head, tail, and solvent characteristics. Hard-core surfactant chains composed of a head segment and three tail segments were simulated in a solvent of hard spheres. The formation of micelles was found to be a strong function of the packing fraction and nonadditivity parameter. Micelles were more stable at higher densities and larger nonadditivity parameters. At lower densities, micelles tended to break into small, dynamic globules.